Summary of Previous Lecture

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{P}_x\right)$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{P}_x\right)$$

$$\Rightarrow$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)$$

$$\hat{P}_x = -i\sqrt{\frac{m\omega\hbar}{2}}\left(\hat{a} - \hat{a}^+\right)$$

$$[\hat{a}, \hat{a}^+] = 1 \qquad \hat{N} = \hat{a}^+\hat{a}$$

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$\hat{H}|n\rangle = \hbar\omega\left(\hat{N} + \tfrac{1}{2}\right)|n\rangle = \underbrace{\hbar\omega\left(n + \tfrac{1}{2}\right)}_{E_n}|n\rangle$$

$$\hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right) \qquad n = 0, 1, 2, \ldots$$

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^+\right)^n|0\rangle$$

Wave functions

$$\langle x|\hat{a}|0\rangle = 0 \qquad \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right)$$

$$\cancel{\sqrt{\frac{m\omega}{2\hbar}}}\langle x|\hat{x} + \frac{i}{m\omega}\hat{p}_x|0\rangle = 0$$

$$\langle x|\hat{x}|0\rangle + \frac{i}{m\omega}\langle x|\hat{p}_x|0\rangle = 0$$

$$\langle x|\hat{x}|0\rangle = x\langle x|0\rangle = x\psi_0(x)$$

$$\langle x|\hat{p}_x|0\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|0\rangle = \frac{\hbar}{i}\frac{d}{dx}\psi_0(x)$$

$$x\psi_0(x) + \frac{i}{m\omega}\cdot\frac{\hbar}{i}\frac{d}{dx}\psi_0(x) = 0 \Rightarrow \frac{d}{dx}\psi_0(x) = -\frac{m\omega}{\hbar}x\psi_0(x)$$

$$\frac{d}{dx}\psi_0(x) = -\frac{m\omega}{\hbar}x\,\psi_0(x)$$

$$\psi_0(x) = N e^{-\frac{m\omega}{2\hbar}x^2}$$

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = |N|^2 \int_{-\infty}^{\infty} e^{-\overset{\alpha}{\frac{m\omega}{\hbar}}x^2} dx = |N|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

$$N = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\langle x|0\rangle = \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}}\langle x|(\hat{a}^+)^n|0\rangle \qquad \hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right)$$

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}}\left(\sqrt{\frac{m\omega}{2\hbar}}\right)^n \langle x|\Big(\underset{\downarrow\, x}{\hat{x}} - \frac{i}{m\omega}\underset{\downarrow\, \frac{\hbar}{i}\frac{d}{dx}}{\hat{p}_x}\Big)^n|0\rangle = \frac{1}{\sqrt{n!}}\left(\sqrt{\frac{m\omega}{2\hbar}}\right)^n\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)^n \psi_0(x)$$

$$\psi_1(x) = \langle x|1\rangle = \langle x|\hat{a}^+|0\rangle = \underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)}_{\hat{a}^+}\underbrace{\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}}_{\psi_0(x)}$$

$$= \frac{1}{\pi^{1/4}\sqrt{2}}\left(\frac{m\omega}{\hbar}\right)^{3/4}\left(x e^{-\frac{m\omega}{2\hbar}x^2} - \frac{\hbar}{m\omega}\frac{d}{dx}e^{-\frac{m\omega}{2\hbar}x^2}\right) = \frac{\sqrt{2}}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4} x e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\Psi_2(x) = \langle x|2\rangle = \frac{1}{\sqrt{2}}\langle x|\hat{a}^+|1\rangle = \frac{1}{\sqrt{2}}\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)}_{\hat{a}^+}\underbrace{\frac{\sqrt{2}}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4} x\, e^{-\frac{m\omega}{2\hbar}x^2}}_{\Psi_1(x)}$$

$$= \frac{1}{\pi^{1/4}\sqrt{2}}\left(\frac{m\omega}{\hbar}\right)^{5/4}\left(x\cdot x e^{-\frac{m\omega}{2\hbar}x^2} - \frac{\hbar}{m\omega}\frac{d}{dx}\left(x e^{-\frac{m\omega}{2\hbar}x^2}\right)\right) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(2\frac{m\omega}{\hbar}x^2 - 1\right)e^{-\frac{m\omega}{2\hbar}x^2}$$

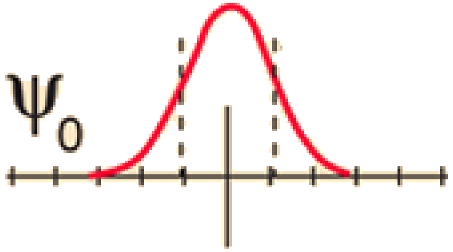
$$\Psi_3(x) = \langle x|3\rangle = \frac{1}{\sqrt{3}}\langle x|\hat{a}^+|2\rangle = \ldots$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi_n(x)=E_n\psi_n(x)$$

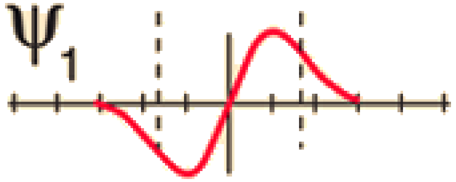
$$E_n=\hbar\omega\left(n+\frac{1}{2}\right)$$

$$n=0,1,2,\ldots$$

$n=0$ $\quad E_0=\frac{\hbar\omega}{2}$ $\quad \psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}$

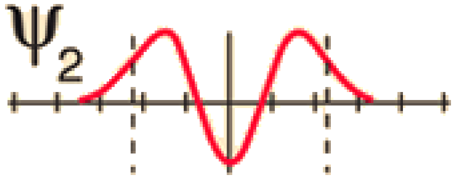


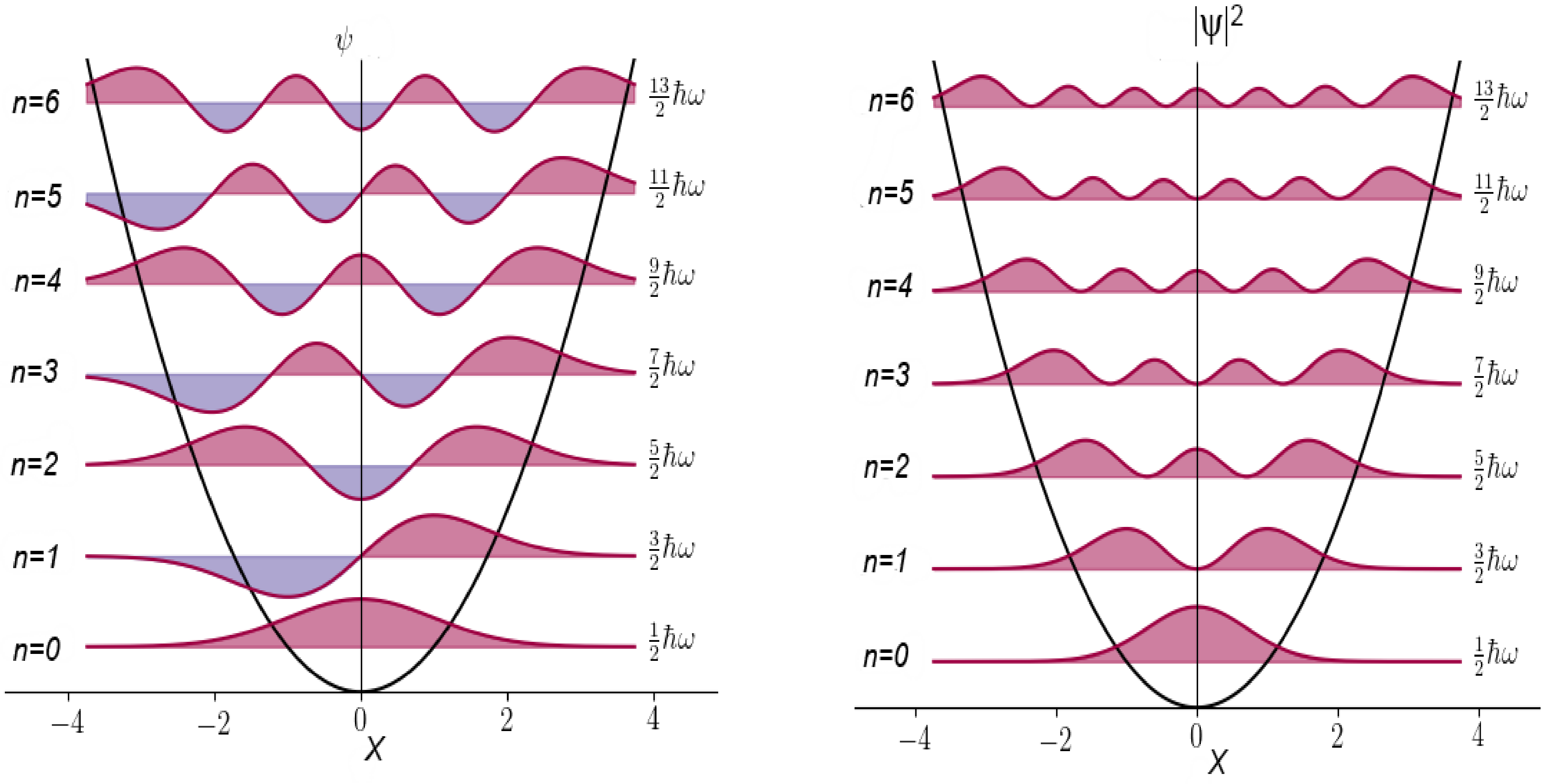
$n=1$ $\quad E_1=\frac{3}{2}\hbar\omega$ $\quad \psi_1(x)=\frac{\sqrt{2}}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4}x\,e^{-\frac{m\omega}{2\hbar}x^2}$



Hermite polynomials

$n=2$ $\quad E_2=\frac{5}{2}\hbar\omega$ $\quad \psi_2(x)=\left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(2\frac{m\omega}{\hbar}x^2-1\right)e^{-\frac{m\omega}{2\hbar}x^2}$





ψ
$|\psi|^2$
n=6
n=5
n=4
n=3
n=2
n=1
n=0
$\frac{13}{2}\hbar\omega$
$\frac{11}{2}\hbar\omega$
$\frac{9}{2}\hbar\omega$
$\frac{7}{2}\hbar\omega$
$\frac{5}{2}\hbar\omega$
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
−4
−2
0
2
4
X

Example 1

For particle in state $|n\rangle$ find ΔX and Δp_x

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+)$$

$$\hat{p}_x = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^+)$$

$$\hat{X}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+)|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$

$$\langle X\rangle = \langle n|\hat{X}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right) = 0$$

$$\langle X^2\rangle = \left(\langle n|\hat{X}\right)\left(\hat{X}|n\rangle\right) = \frac{\hbar}{2m\omega}\left(\sqrt{n}\,\langle n-1| + \sqrt{n+1}\,\langle n+1|\right)\left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$

$$\langle X^2\rangle = \frac{\hbar}{2m\omega}(n + (n+1)) = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right) \Rightarrow \Delta X = \sqrt{\langle X^2\rangle - \langle X\rangle^2} = \sqrt{\frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)}$$

$$\hat{p}_x = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^+)$$

$$\hat{p}_x|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^+)|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n}|n-1\rangle - \sqrt{n+1}|n+1\rangle\right)$$

$$\langle p_x\rangle = \langle n|\hat{p}_x|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}\langle n|\left(\sqrt{n}|n-1\rangle - \sqrt{n+1}|n+1\rangle\right) = 0$$

$$\langle p_x^2\rangle = (\langle n|\hat{p}_x)(\hat{p}_x|n\rangle) = \frac{m\omega\hbar}{2}\left(\sqrt{n}\langle n-1| - \sqrt{n+1}\langle n+1|\right)\left(\sqrt{n}|n-1\rangle - \sqrt{n+1}|n+1\rangle\right)$$

$$\langle p_x^2\rangle = \frac{m\omega\hbar}{2}(n+(n+1)) = m\omega\hbar\left(n+\frac{1}{2}\right)$$

$$\Delta p_x = \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2} = \sqrt{m\omega\hbar\left(n+\frac{1}{2}\right)}$$

$$\Delta x \Delta p_x = \hbar(n + 1/2)$$

Example 2

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|2\rangle + \frac{i}{\sqrt{2}}|4\rangle$$

$$\langle E\rangle = \frac{1}{2}\cdot\hbar\omega\left(2+\frac{1}{2}\right) + \frac{1}{2}\hbar\omega\left(4+\frac{1}{2}\right) = \frac{7}{2}\hbar\omega$$

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-\frac{iE_2 t}{\hbar}}|2\rangle + \frac{i}{\sqrt{2}}e^{-\frac{iE_4 t}{\hbar}}|4\rangle$$

$$= \frac{1}{\sqrt{2}}e^{-i\omega\left(2+\frac{1}{2}\right)t}|2\rangle + \frac{i}{\sqrt{2}}e^{-i\omega\left(4+\frac{1}{2}\right)t}|4\rangle = e^{-i\frac{5}{2}\omega t}\left(\frac{1}{\sqrt{2}}|2\rangle + \frac{i}{\sqrt{2}}e^{-2i\omega t}|4\rangle\right)$$

1) $\langle E\rangle$ - ?
2) $|\Psi(t)\rangle$ - ?
3) $\langle x\rangle$ - ?
4) $\langle x^2\rangle$ - ?
5) $\langle V\rangle$ - ?
6) $\langle K\rangle$ - ?

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}|2\rangle + \frac{i}{\sqrt{2}}e^{-2i\omega t}|4\rangle$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})$$

$$\hat{x}|\psi(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})\left(\frac{1}{\sqrt{2}}|2\rangle + \frac{i}{\sqrt{2}}e^{-2i\omega t}|4\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{\sqrt{2}}\sqrt{2}|1\rangle + \frac{i}{\sqrt{2}}e^{-2i\omega t}\sqrt{4}|3\rangle + \frac{1}{\sqrt{2}}\sqrt{3}|3\rangle + \frac{i}{\sqrt{2}}e^{-2i\omega t}\sqrt{5}|5\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(|1\rangle + \left(i\sqrt{2}e^{-2i\omega t} + \sqrt{\frac{3}{2}}\right)|3\rangle + i\sqrt{\frac{5}{2}}e^{-2i\omega t}|5\rangle\right)$$

$$\langle X\rangle = \langle\psi|\hat{X}|\psi\rangle = \underbrace{\left(\frac{1}{\sqrt{2}}\langle 2| - \frac{i}{\sqrt{2}}e^{2i\omega t}\langle 4|\right)}_{\langle\psi(t)|}\underbrace{\sqrt{\frac{\hbar}{2m\omega}}\left(|1\rangle + \left(i\sqrt{2}e^{-2i\omega t} + \sqrt{\frac{3}{2}}\right)|3\rangle + i\sqrt{\frac{5}{2}}e^{-2i\omega t}|5\rangle\right)}_{\hat{x}|\psi(t)\rangle} = 0$$

$$\langle X^2\rangle = \left(\langle\psi(t)|\hat{X}\right)\left(\hat{X}|\psi(t)\rangle\right) = \frac{\hbar}{2m\omega}\left(\langle 1| + \left(-i\sqrt{2}\,e^{2i\omega t} + \sqrt{\tfrac{3}{2}}\right)\langle 3| - i\sqrt{\tfrac{5}{2}}\,e^{2i\omega t}\langle 5|\right)\cdot$$

$$\cdot\left(|1\rangle + \left(i\sqrt{2}\,e^{-2i\omega t} + \sqrt{\tfrac{3}{2}}\right)|3\rangle + i\sqrt{\tfrac{5}{2}}\,e^{-2i\omega t}|5\rangle\right)$$

$$= \frac{\hbar}{2m\omega}\left(1 + \left(-i\sqrt{2}\,e^{2i\omega t} + \sqrt{\tfrac{3}{2}}\right)\left(i\sqrt{2}\,e^{-2i\omega t} + \sqrt{\tfrac{3}{2}}\right) + \frac{5}{2}\right)$$

$$= \frac{\hbar}{2m\omega}\left(1 + 2 - i\sqrt{3}\,e^{2i\omega t} + i\sqrt{3}\,e^{-2i\omega t} + \frac{3}{2} + \frac{5}{2}\right)$$

$$= \frac{\hbar}{2m\omega}\left(7 + 2\sqrt{3}\,\frac{e^{2i\omega t} - e^{-2i\omega t}}{2i}\right) = \frac{\hbar}{2m\omega}\left(7 + 2\sqrt{3}\sin 2\omega t\right)$$

$$\hat{V} = \frac{1}{2} m\omega^2 \hat{x}^2$$

$$\langle V \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle = \frac{1}{2} m\omega^2 \cdot \frac{\hbar}{2m\omega} \left(7 + 2\sqrt{3} \sin 2\omega t\right) = \frac{\hbar\omega}{4}\left(7 + 2\sqrt{3} \sin 2\omega t\right)$$

$$\langle E \rangle = \langle K \rangle + \langle V \rangle \quad \Rightarrow \quad \langle K \rangle = \langle E \rangle - \langle V \rangle$$

$$\langle K \rangle = \underbrace{\frac{7}{2}\hbar\omega}_{\langle E \rangle} - \underbrace{\frac{\hbar\omega}{4}\left(7 + 2\sqrt{3} \sin 2\omega t\right)}_{\langle V \rangle} = \frac{\hbar\omega}{4}\left(7 - 2\sqrt{3} \sin 2\omega t\right)$$

E_n and $\psi_n(x)$ for particle confined in arbitrary $V(x)$

1) analytic solution: eg. $\psi(x) = \sum_{k=0}^{\infty} c_k x^k$

2) Numerical Solution Finite Difference Method

https://en.wikipedia.org/wiki/Finite_difference_method

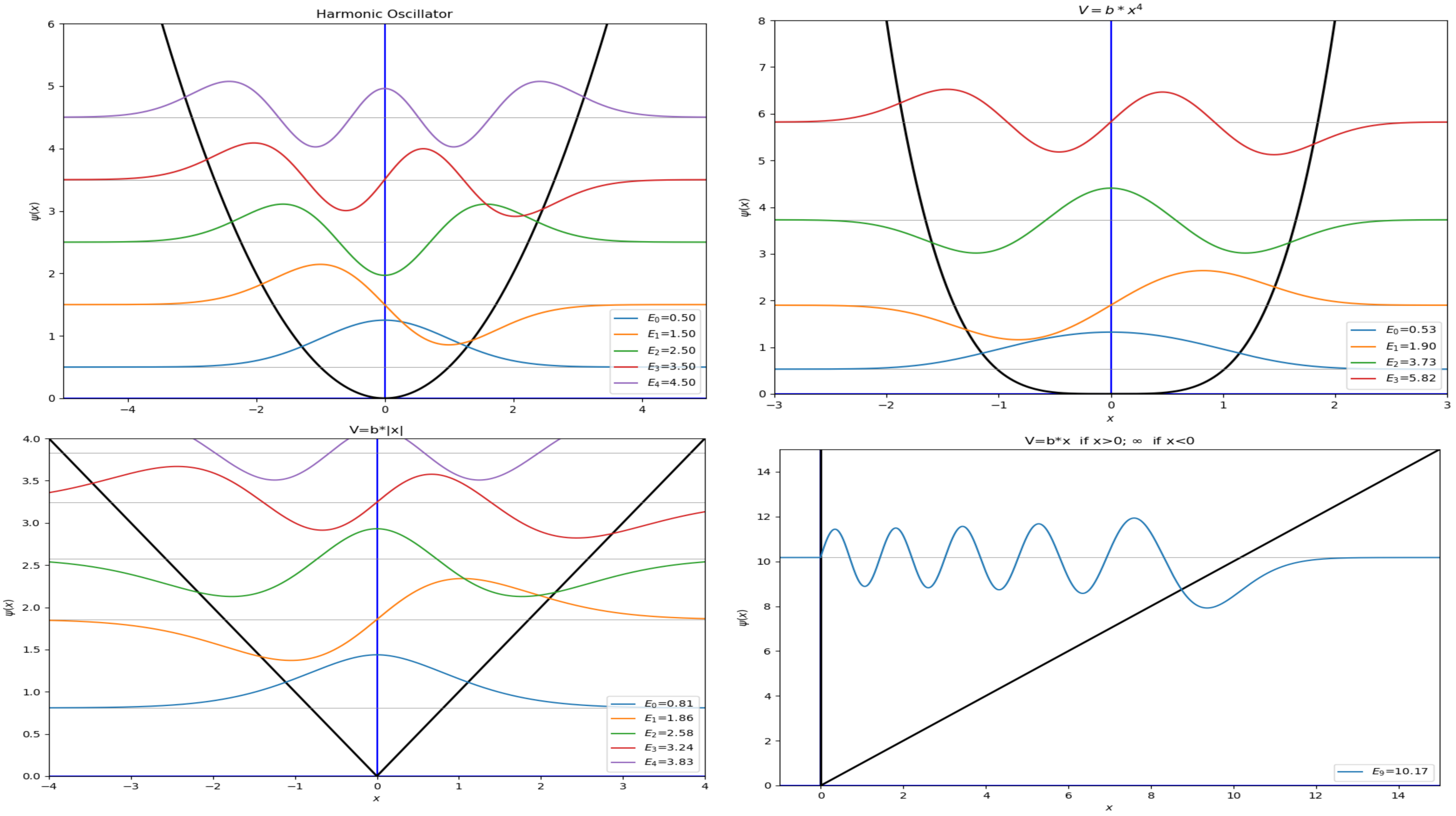
$$X = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} \qquad \psi(x) = \begin{pmatrix} \psi(x_0) \\ \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{pmatrix}$$

$$\mathbf{H} = \frac{-\hbar^2}{2mh^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \\ 1 & -2 & 1 & 0 & \\ 0 & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 \end{pmatrix} + \begin{pmatrix} V_0 & 0 & 0 & & \\ 0 & V_1 & 0 & & \\ 0 & 0 & V_2 & & \\ & & & \ddots & \\ & & & & V_{N-1} \end{pmatrix}$$

$h = x_{i+1} - x_i$

$$\hat{H}\psi = E\psi$$

https://github.com/mholtrop/QMPython


Harmonic Oscillator
ψ(x)
E_0=0.50
E_1=1.50
E_2=2.50
E_3=3.50
E_4=4.50
$V = b * x^4$
ψ(x)
x
E_0=0.53
E_1=1.90
E_2=3.73
E_3=5.82
V=b*|x|
ψ(x)
x
E_0=0.81
E_1=1.86
E_2=2.58
E_3=3.24
E_4=3.83
V=b*x if x>0; ∞ if x<0
ψ(x)
x
E_9=10.17